(*2*). In my Research Commentary, I did refer to this later paper, but as it does not contain experimental results, I agree that I should have also referred to the original paper (*1*).

Whether the system of Fahmy *et al.* constitutes a true quantum computer is open to debate, as they implemented quantum gates, but apparently did not attempt to implement quantum algorithms. They did, however, demonstrate all the basic elements required to build such a computer and therefore could be called the "fathers" of the NMR quantum computer. I am delighted to have this opportunity to clarify the matter.

Jonathan A. Jones
Oxford Centre for Molecular Sciences, New Chemistry Laboratory, South Parks Road, Oxford OX1 3QT, United Kingdom. E-mail: jones@bioch.ox.ac.uk

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Crystallography of a Photocycle Intermediate

In their report "Energy transduction on the nanosecond time scale: Early structural events in a xanthopsin photocycle" (20 Mar., p. 1946), Benjamin Perman *et al.* discuss how proteins change when light energy is converted into a chemical signal in a halophilic phototrophic bacterium (*1*). It seems to us, however, that the crystallography in the report is in error. The most serious problem is that the proposed structure of the intermediate does not agree with the difference electron density map. The largest negative electron density feature (M) is appropriately ascribed to movement of the carbonyl oxygen, but the large positive density (L), which would logically be associated with the carbonyl, is incorrectly ascribed to movement of the carbon-carbon double bond.

The results reported by Perman *et al.* should be compared with those of Genick *et al.* (*2*), which was also about a photoactive yellow protein photocycle early intermediate (*3*). The differences that are present may be ascribed to a lower resolution of the data in the report by Perman *et al.*, which in our view has led to an incorrect interpretation. The higher resolution results obtained by Genick *et al.* (*2*), during isomerization of the carbon-carbon double bond, show that it is the carbonyl group that rotates.

T. E. Meyer
G. Tollin
M. A. Cusanovich
Department of Biochemistry, University of Arizona, Tucson, AZ 85721, USA. E-mail: gtollin@u.arizona.edu

References and Notes

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2. U. K. Genick *et al.*, *Nature* **392**, 206 (1998).
3. We also prefer the nomenclature used by Genick *et al.* (*2*) and established earlier by our group (*1*) to that used in the report by Perman et al.; that is, photoactive yellow protein, not xanthopsin, and intermediates I^1 and I^2, instead of pR and pB.

Response

Meyer *et al.* raise an interesting point concerning the structural interpretation presented in our report, which was derived from real-time, ambient temperature measurements, in contrast with that derived from data obtained at cryogenic temperature by Genick *et al.* (*1*). These interpretations unquestionably differ. The interpretation of our results now advanced by the Arizona group was in fact the one we considered first immediately on inspecting our results. In our initial attempts, the intermediate did not behave as well under crystallographic refinement as the one we presented in our report. When we became aware of the Genick *et al.* results [one of us (K.M.) and Elizabeth Getzoff presented their results back-to-back at a meeting in Grenoble, France, in January 1998], we reexamined our structural interpretation and concluded that our crystallographic data was not compatible with the model proposed by Genick *et al.*

It is possible for the interpretations in both our report and in the paper by Genick *et al.* (*1*) to be correct because the conditions under which the data were obtained are so different. Structural relaxation is greatly hindered at cryogenic temperatures and may be qualitatively (not just quantitatively) altered from that at ambient temperature. Freeze-trapping of authentic reaction intermediates is therefore not necessarily a straightforward process (*2*). Related studies, from our laboratory, of time-resolved crystallography on myoglobin at both ambient and cryogenic temperatures (*3*) also encounter this question. We maintain that our data and interpretation are correct (*4*).

Benjamin Perman
Department of Biochemistry and Molecular Biology, University of Chicago, Chicago, IL 60637, USA
Michael Wulff
European Synchrotron Radiation Facility, 38043 Grenoble Cedex, France
Klaas Hellingwerf
Laboratory for Microbiology, University of Amsterdam, 1018 WS Amsterdam, Netherlands
Keith Moffat
Department of Biochemistry and Molecular Biology and Consortium for Advanced Radiation Sources, University of Chicago

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4. "Xanthopsins" refers to the family of photoactive yellow proteins [R. Kort *et al.*, *EMBO J.* **15**, 3209 (1996)].